LINEAR MODELS FOR CLASSIFICATION (PART 1)

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Topics

- Introduction
- Discriminant Function

- Probabilistic Discriminative Models

- Laplace Approximation
- Bayesian Logistic Regression

INTRODUCTION

Introduction

- Regression:
  - Map input vector x to one or more continuous target variables t
- Classification:
  - Map input vector x to one of K discrete classes ($K \geq 2$)
- Ordinal Regression:
  - Map input vector x to one of K discrete classes that have an ordering (e.g., on-line evaluation (stars))

Linear Classification Models

- Simple scenario: disjoint classes
- Divide input space into decision regions
- Linear model decision surface are linear function of input x
  - D-1 dimension hyperplane in D dimensional input space
- Linearly separable:
  - Classes in a dataset can be separated exactly using linear decision surface

Probabilistic Models

- Converting Regression to Class Output
- Target variables *t* now represent class labels
- Binary class representation is convenient
  - Two classes: $t \in \{0,1\}$, t=1 represent C_1; t=0 represent C_0
  - Interpret value of *t* as the probability that class is C_1
  - Probabilities need to take value between 0 and 1
  - For K>2, use 1-of-K coding scheme
    - E.g. K=5, $t = (0,1,0,0,0)^T$ represents class 2
    - Value t_k interpreted as probability of class C_k

Two Approaches to Classification

- Discriminant function
  - Directly assign x to a specific class
  - E.g. Fisher's linear discriminant function, perceptron
- Probabilistic models
  - Model $p(C_k|x)$ and make optimal decisions
- Probabilistic models separating inference from decision
  - Accommodate different loss function
  - Compensate for unbalanced data
  - Combine models

Probabilistic Classification Models

- Generative
  - Model class conditional densities by $p(x|C_k)$ together with prior probabilities $p(C_k)$
  - $p(C_k|x) \propto p(x|C_k)p(C_k)$

- Discriminative
  - Directly model conditional probabilities $p(C_k|x)$

Converting Linear Regression Models to Linear Classification Models

- Linear regression model y(x,w) is a linear function of parameters w
- In simplest case also a linear function of variable x
  - $y(x) = w^T x + w_0$
- For classification we wish to obtain a discrete output or posterior probabilities in range (0,1)
- Use generalization of this model $y(x) = f(w^T x + w_0)$
  - $f(\cdot)$ is an activation function
  - $f^{-1}(\cdot)$ is a link function

Generalized Linear Model

- $y(x) = f(w^T x + w_0)$
- The decision surface correspond to $y(x) = constant$ or $w^T x + w_0$=constant
- So decision boundaries are linear even if $f(\cdot)$ is nonlinear
  - ➔Generalized Linear Model
- No longer linear w.r.t to w due to $f(\cdot)$
  - Lead to more complex models for classification than regression

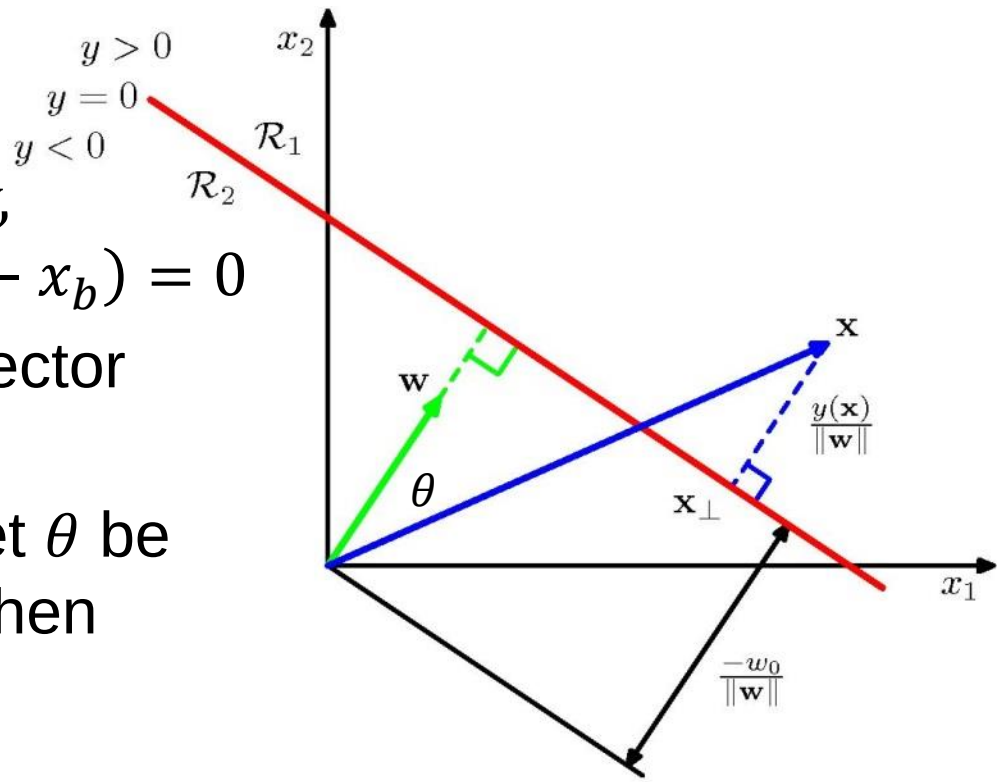
DISCRIMINANT FUNCTIONS

Linear Discriminant Function

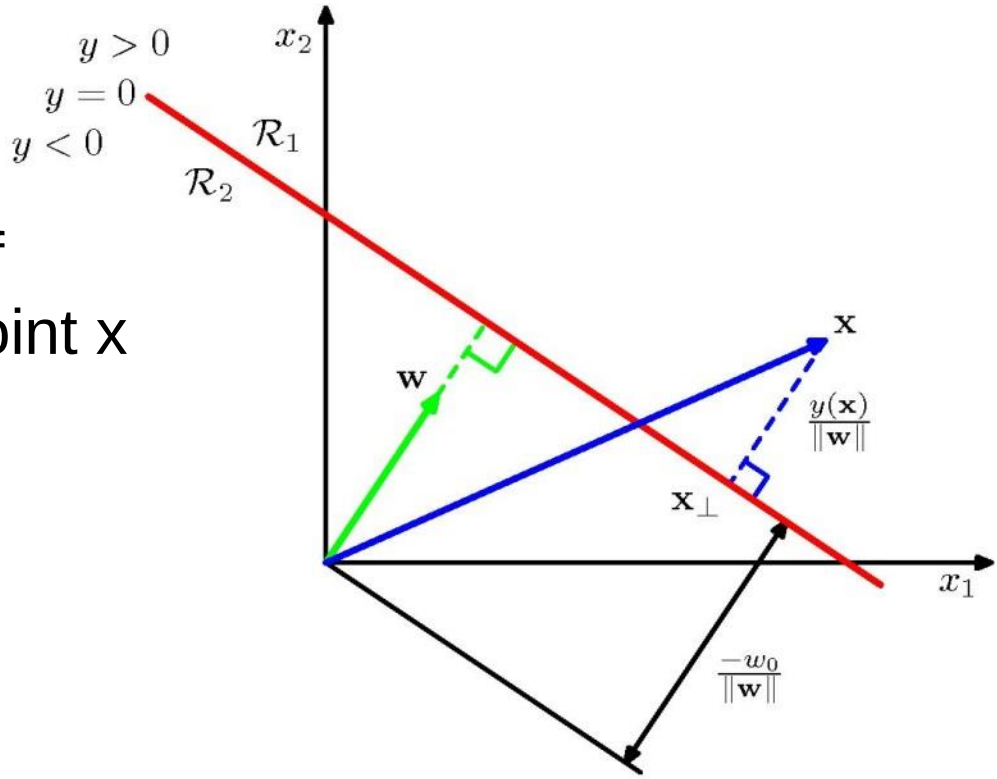
- Assigns input vector x to one of K classes denoted by C_k
- Restrict attention to linear discriminants (decision hyperplanes)
- Two-class linear discriminant function:
  - $y(x) = w^T x + w_0$
  - w is a weight vector and w_0 is bias
  - Assign x to C_1 if $y(x) \geq 0$, else C_2

Geometry of Linear Discriminant Functions

- $y(x) = w^T x + w_0$
- Decision boundary: $y(x) = 0$
- For x_a and x_b on the boundary, $y(x_a) - y(x_b) = 0$, ➔ $w^T(x_a - x_b) = 0$
- ➔ w is orthogonal to every vector on surface.
- Given an arbitrary vector x, let θ be the angle between x and w, then $\cos\theta = \frac{x \cdot w}{\|x\|\|w\|}$
- The projection length of x on w is $\|x\|\cos\theta = \frac{w^T x}{\|w\|} = \frac{y(x) - w_0}{\|w\|} = \frac{y(x)}{\|w\|} + \frac{-w_0}{\|w\|}$



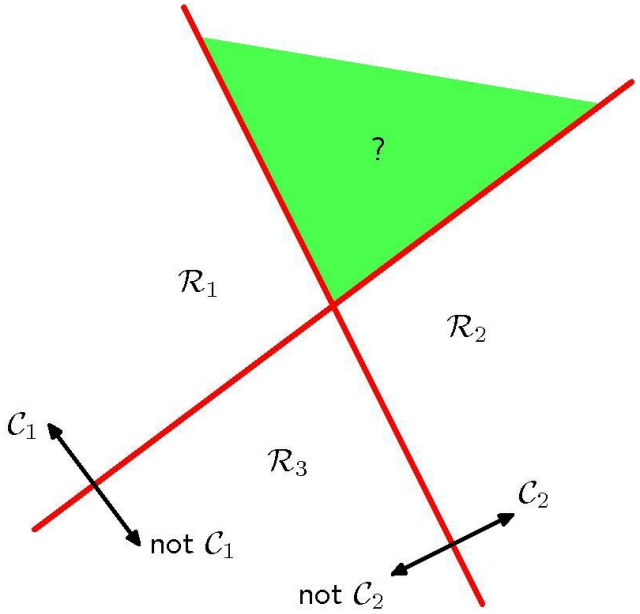
Geometry of Linear Discriminant Functions



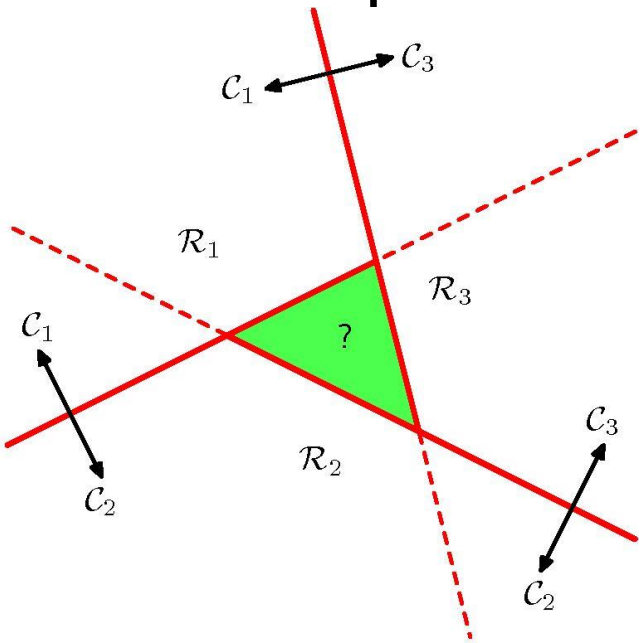
- $y(x) = w^T x + w_0$
- $y(x)$ gives signed measure of perpendicular distance r of point x to decision surface ($r = \frac{y(x)}{\|w\|}$)
- w_0 sets distance of origin to surface ($\frac{y(0)}{\|w\|} = \frac{w_0}{\|w\|}$)
- With dummy input $x_0 = 1$, and $\omega = (w_0, w^T)^T$, $z = (x_0, x^T)^T$, then $y(x) = \omega^T z$
  - Pass through origin in augmented D+1 dimensional space

Multiple Classes with 2-class classifiers

- One-versus-the-rest
- Build a K class discriminant using K-1 classifiers



- One-versus-one
- Build K(K-1)/2 binary discriminant classifiers, one for each pair



Both result in ambiguous regions of input space

Multiple Classes with K Discriminants

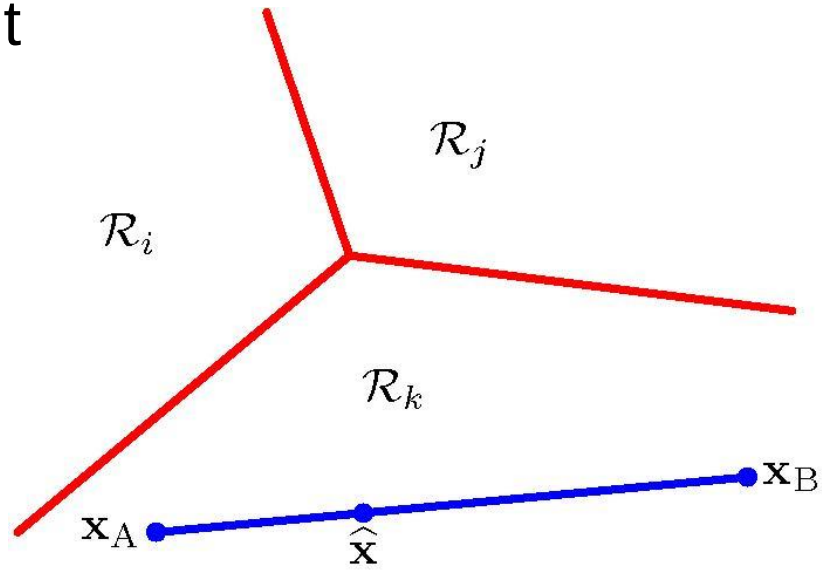
- Consider a single K class discriminants of the form
  - $y_k(x) = w_k^T x + w_{k0}, \; k = 1,2, \ldots, K$
  - Assign a point x to class C_k if $y_k(x) > y_j(x)$ for all $j \neq k$
- Decision boundary between class C_k and C_j is given by $y_k(x) = y_j(x)$
  - Corresponds to D-1 dimensional hyperplane defined by

$$\left(w_k - w_j\right)^T x + \left(w_{k0} - w_{j0}\right) = 0$$

  - Same form as the decision boundary for 2-class case
  - Decision regions of such a discriminant are always singly connected and convex
    - Proof on next slide

Convexity of Decision Regions

- Consider two points x_a and x_b both in decision region R_k
- Any point $\hat{x}$ on line connecting x_a and x_b can be expressed as $\hat{x} = \lambda x_a + (1-\lambda)x_b$, where $0 \leq \lambda \leq 1$.
- From linearity of discriminant functions $y_k(x) = w_k^T x + w_{k0}$
- Combining the two, we have $y_k(\hat{x}) = \lambda y_k(x_a) + (1-\lambda) y_k(x_b)$
- Because x_a and x_b lie inside R_k, it follows that $y_k(x_a) > y_j(x_a)$ and $y_k(x_b) > y_j(x_b)$ for all $j \neq k$.
- Hence $\hat{x}$ also lies inside R_k
- Thus R_k is singly-connected and convex



Learning the Parameters of Linear Discriminant Functions

- Three methods
  - Least squares
  - Fisher's Linear Discriminant (omitted)
  - Perceptrons

Least Square for Classification

- Simple closed-form solution exists
- Each C_k, $k = 1,2, \ldots, K$, is described by its own linear model

$$y_k(x) = w_k^T x + w_{k0}$$

- Create augmented vector $x = (1, x^T)^T$ and $w_k = \left(w_{k0}, w_k^T\right)^T$ (length is D+1)
- Grouping into vector notation $y(x) = W^T x$
  - W is the parameter matrix whose kth column is a D+1 dimensional vector (including bias)
  - $W = [w_1\ w_2\ \ldots w_K]$
  - $y(x)$ is K by 1
- New input vector x is assigned to class for which output $y_k = w_k^T x$ is largest
- Determine W by minimizing squared error

Learning Parameters Using Least Squares

- Training data $\{x_n, t_n\}$, $n = 1,2, \ldots, N$.
  t_n is a column vector of K dimensions using 1-of-K form
- Define matrices

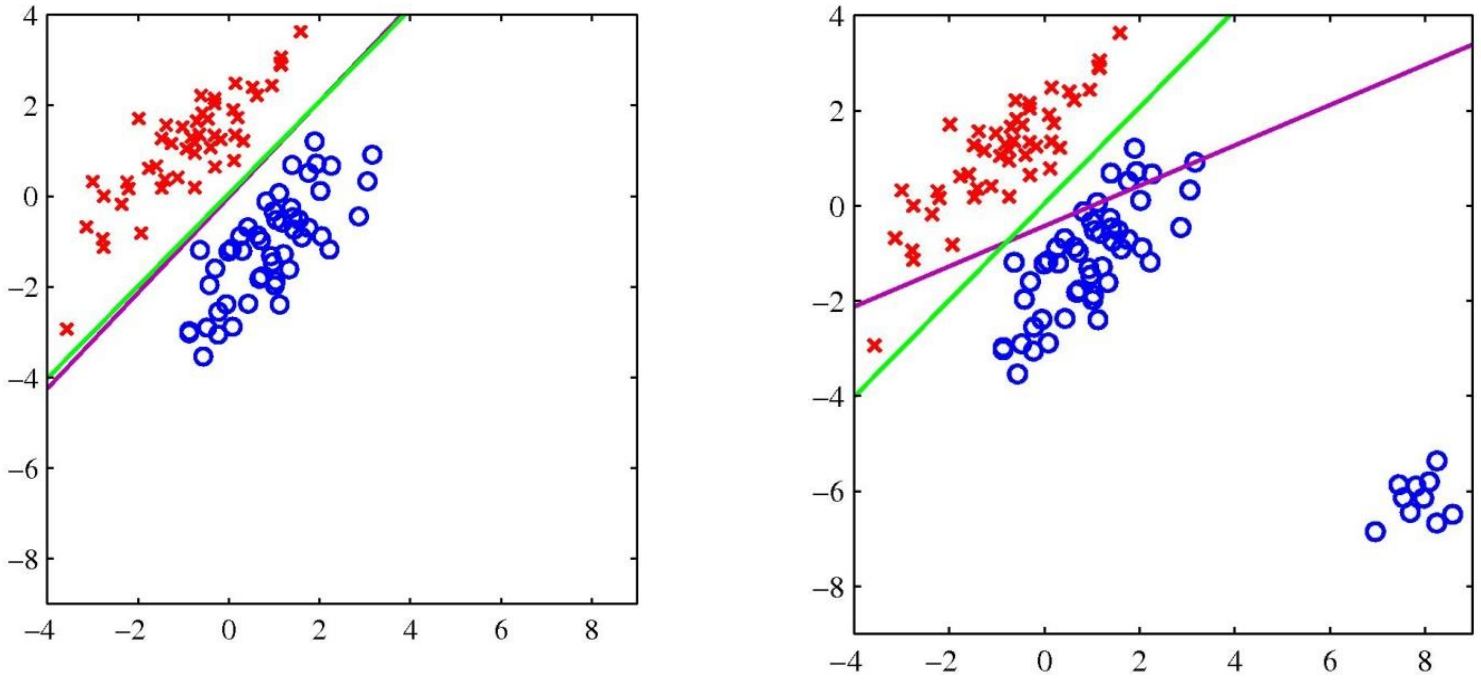
$$T = \begin{bmatrix} t_1^T \\ t_2^T \\ \vdots \\ t_N^T \end{bmatrix}, X = \begin{bmatrix} x_1^T \\ x_2^T \\ \vdots \\ x_N^T \end{bmatrix}, \text{ Error vector} = \underset{N \times (D+1)}{X} \underset{(D+1) \times K}{W} - \underset{N \times K}{T}$$

- Let $B = XW - T = \begin{bmatrix} e_1^T \\ e_2^T \\ \vdots \\ e_N^T \end{bmatrix}$, we are trying to minimize the sum of squared errors $\sum_{j=1}^{K} \sum_{i=1}^{N} e_{ij}^2$.

Learning Regression Parameters

- We have k vectors to learn: $W = [w_1\ w_2\ \ ...\ w_K]$
- Each w_i controls the $i - th$ dimension of the output.
- All of the K vectors can be learned separately.
- That is, we can learn K separate regression models, each use one of the K columns in T as the outcome vector in the linear regression models we introduced before.
- To predict the output class for an input x, compute $y_i = w_i^T x$ for $i = 1, 2, ..., K$, and
- classify x to class k for which y_k is the maximum.

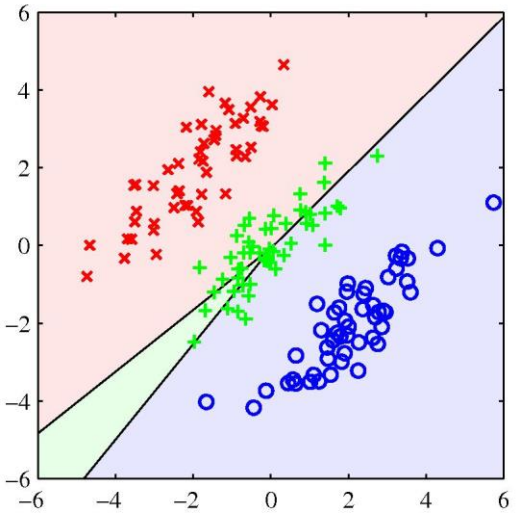
[Limitation] Least Square is Sensitive to Outliers

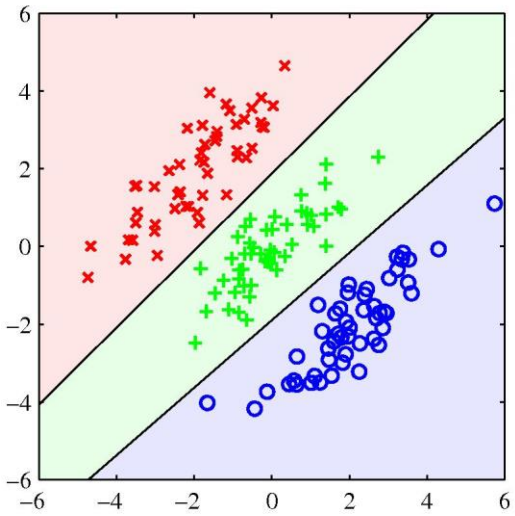


- Sum of squared errors penalized predictions that are “too correct” (magenta lines)
  - Long way from decision boundary
  - Logistic regression (green lines) does not have this problem
  - SVMs have an hinge error function that have a similar shape to that of the logistic regression

Disadvantages of Least Squares

Ordinary regression





Logistic regression

- Regions assigned to green class is too small, mostly misclassified
- Logistic regression performs well
- Disadvantage of least square:
  - Lack robustness to outliers
  - Gaussian assumption may not be a good choice for classification problems
  - Binary target values have a distribution far from Gaussian

Perceptron Algorithm

- Two-class model
  - Input vector x transformed by a fixed nonlinear function to give feature vector $\phi(x)$
  - $y(x) = f(w^T \phi(x))$
    where non-linear activation $f(\cdot)$ is a step function
  - $f(a) = \begin{cases} +1 \; if \; a \geq 0 \\ -1 \; if \; a < 0 \end{cases}$
- Use a target coding scheme
  - t=1 for class C_1, and t=-1 for C_2 similar to the activation function

Perceptron Error Function

- Error function: number of misclassifications
- This error function is a piecewise constant function of *w* with discontinuities (unlike regression)
- Hence no closed form solution

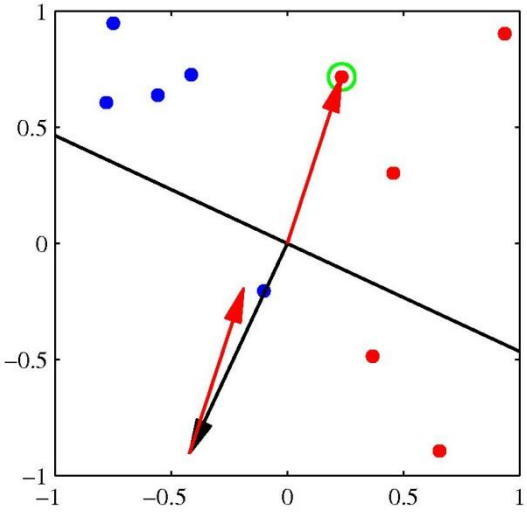
Perceptron Criterion

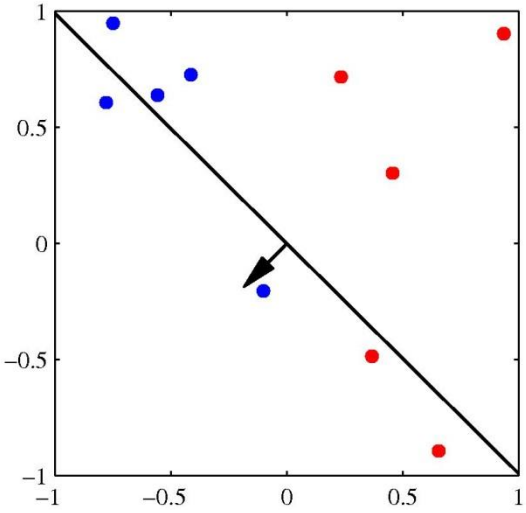
- Seek w such that $x_n \in C_1$ will have $w^T x_n \geq 0$ where as $x_n \in C_2$ will have $w^T x_n < 0$
- Target value $t \in \{-1, 1\}$. C_1 ➔ t=1, all patterns need to satisfy $w^T \phi(x_n) t_n > 0$
- For each misclassified sample, perceptron criterion tried to minimize $E_p(w) = -\sum_{n \in \mathrm{M}} w^T \phi_n t_n$
- M denotes set of all misclassified patterns and $\phi_n = \phi(x_n)$

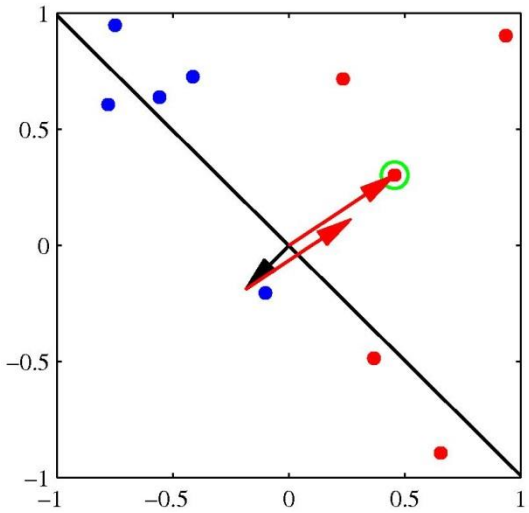
Perceptron Algorithm

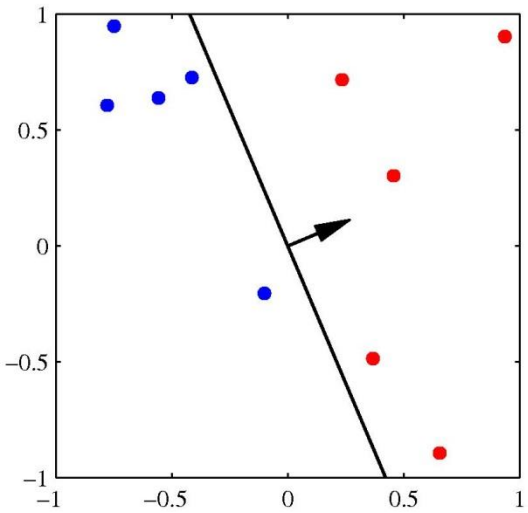
- Error function $E_p(w) = -\sum_{n\in \mathrm{M}} w^T \phi_n t_n \equiv \sum_{n\in M} E_n$
- **Stochastic gradient descent**
  - a.k.a Sequential gradient descent
  - Loop through M, for each data point n, change in weight is given by
  - $w^{\tau+1} = w^{\tau} - \eta \nabla \mathrm{E_n(w)} = w^{\tau} + \eta \phi_n t_n$
  - $\nabla E_n(w) = \frac{\partial E_n(w)}{\partial w} = -\phi_n t_n$
    η is learning rate (set to 1), τ is a step index
- The algorithm
  - Cycle through the training patterns in turn
  - If incorrectly classified for class C_1, add to weight vector
  - If incorrectly classified for class C_2, subtract from weight vector

Perceptron Learning



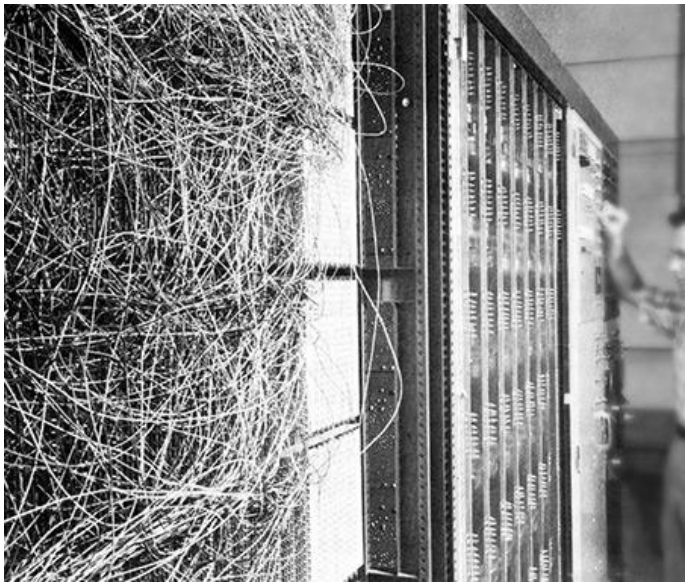






- Green point is misclassified ➔ add to weight vector (black arrow)

History of Perceptron



- Perceptron invented by Frank Rosenblatt
- Mark 1 perceptron hardware (patching board, allowing different configurations)

Disadvantages of Perceptrons

- Does not converge if classes not linearly separable
- Does not provide probabilistic output
- Not readily generalized to K>2 classes

Comparison of Parameter Learning Approaches

- Least Squares
  - Not robust to outliers, model close to target values
- Fisher's linear discriminant (omitted)
  - Separation determined by within-class and between class variance
  - Can be seen as a special case of least square
- Perceptrons
  - Does not converge if classes not linearly separable
  - Does not provide probabilistic output
  - Not readily generalized to K>2 classes

QUESTIONS?